Down to the metal with scikit-learn

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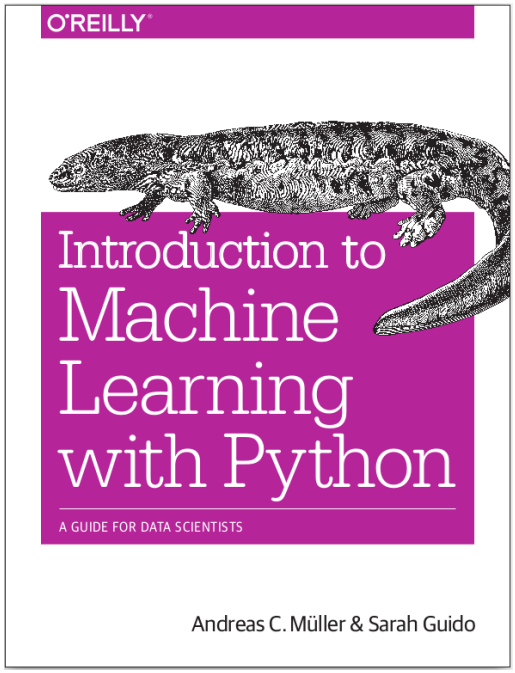
Amazon Machine Learning

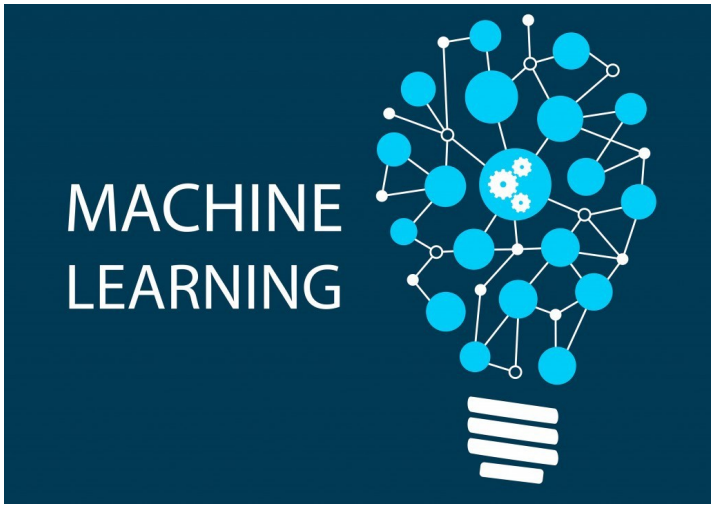


NYU Center for Data Science

COLUMBIA UNIVERSITY
Data Science Institute

What is scikit-learn?


python


MACHINE
LEARNING

Classification
Regression
Clustering
Semi-Supervised Learning
Feature Selection
Feature Extraction
Manifold Learning
Dimensionality Reduction
Kernel Approximation
Hyperparameter Optimization
Evaluation Metrics
Out-of-core learning
……

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Mission

Commoditize and Democratize Machine Learning

Basic API

Representing Data

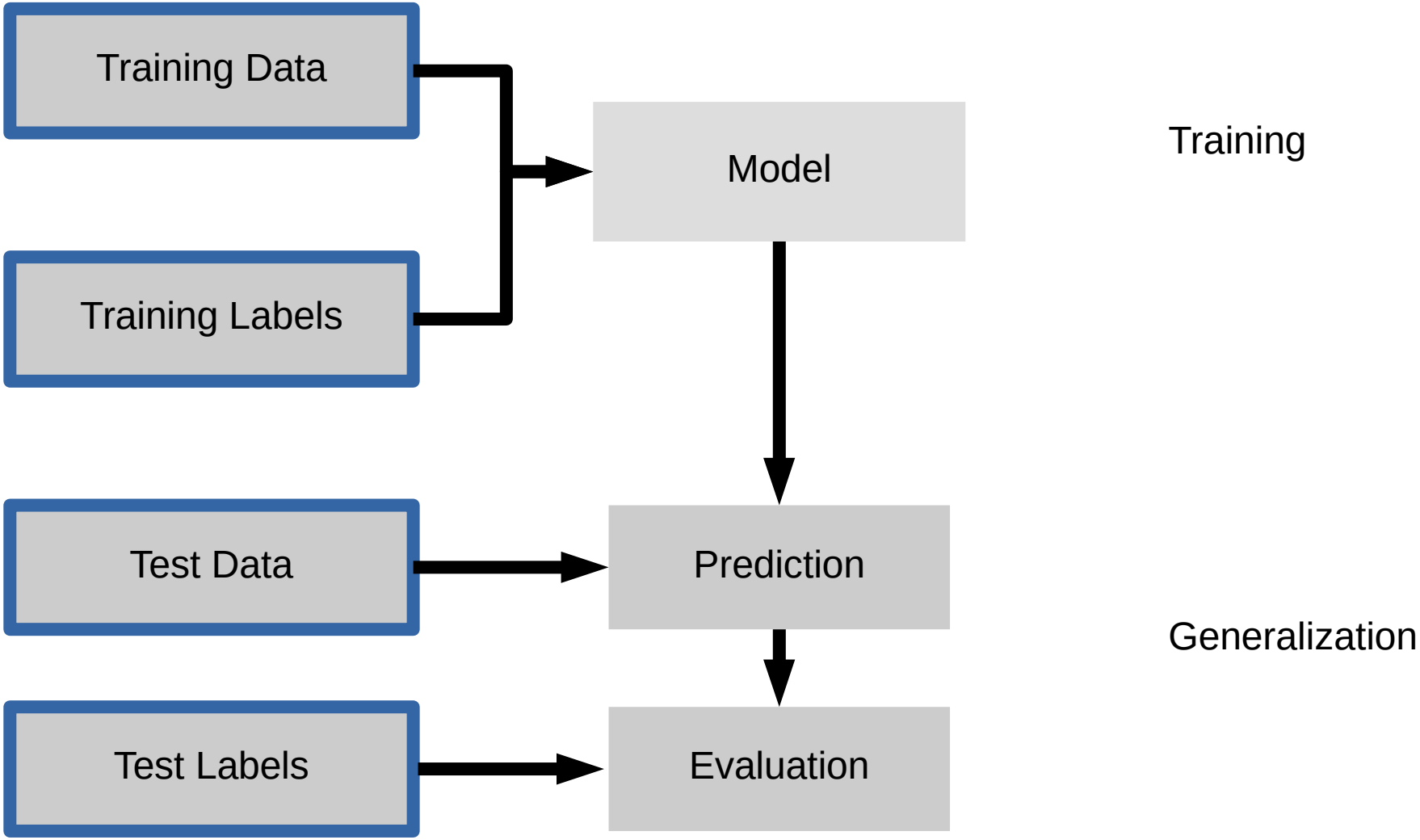
one sample

$$X = \begin{pmatrix} 1.1 & 2.2 & 3.4 & 5.6 & 1.0 \\ 6.7 & 0.5 & 0.4 & 2.6 & 1.6 \\ 2.4 & 9.3 & 7.3 & 6.4 & 2.8 \\ 1.5 & 0.0 & 4.3 & 8.3 & 3.4 \\ 0.5 & 3.5 & 8.1 & 3.6 & 4.6 \\ 5.1 & 9.7 & 3.5 & 7.9 & 5.1 \\ 3.7 & 7.8 & 2.6 & 3.2 & 6.3 \end{pmatrix} \qquad y = \begin{pmatrix} 1.6 \\ 2.7 \\ 4.4 \\ 0.5 \\ 0.2 \\ 5.6 \\ 6.7 \end{pmatrix}$$

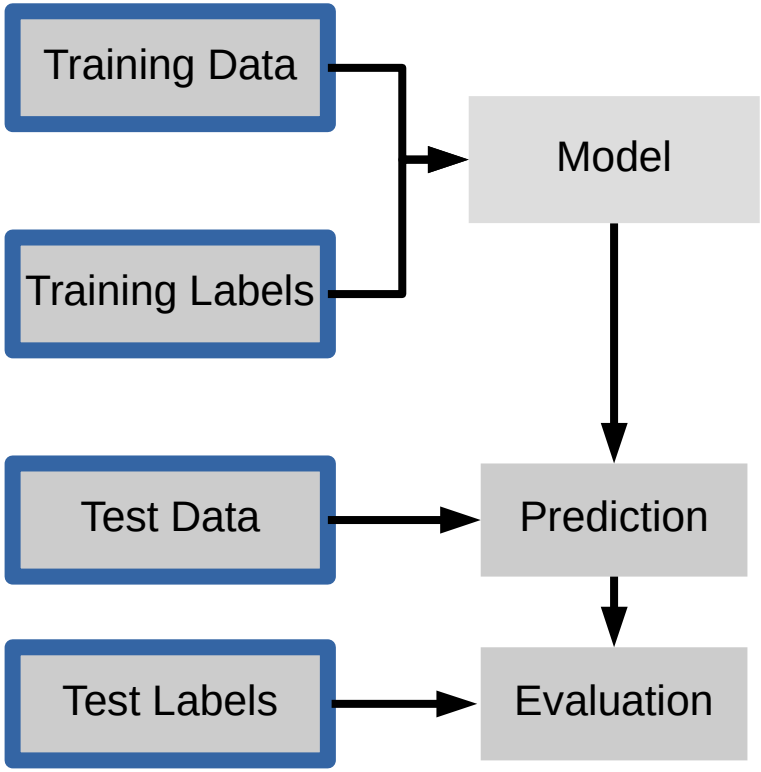
one feature

outputs / labels

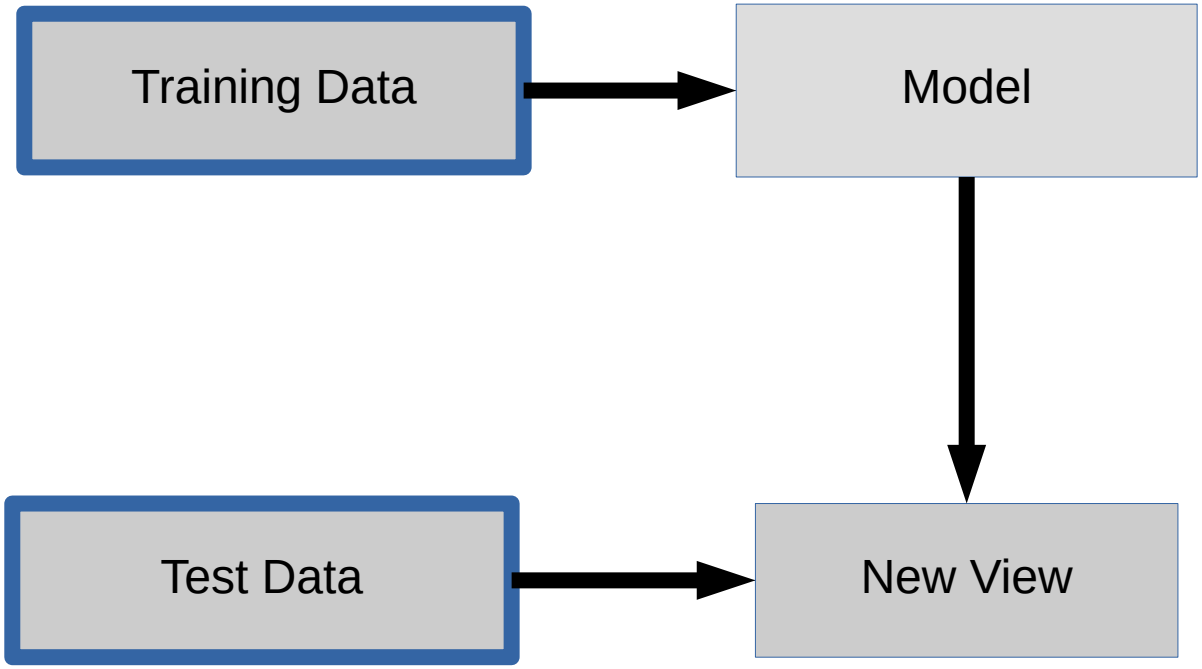
Supervised Machine Learning



```
clf = RandomForestClassifier()

clf.fit(X_train, y_train)

y_pred = clf.predict(X_test)

clf.score(X_test, y_test)
```

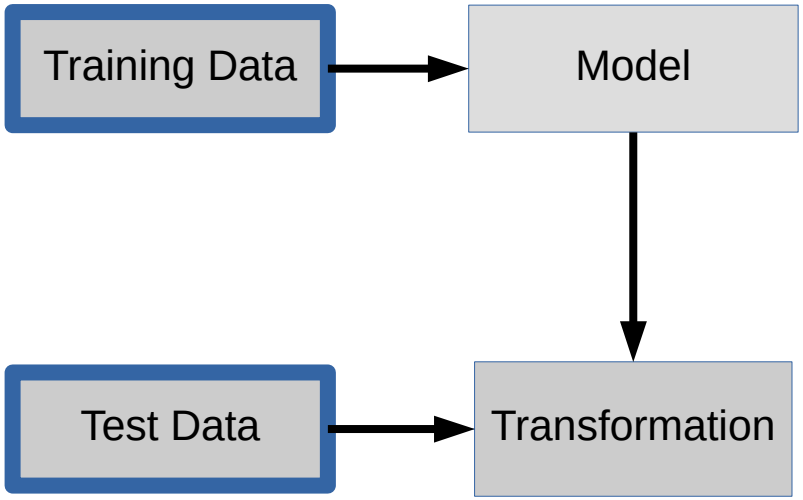


Unsupervised Machine Learning



Unsupervised Transformations

```
pca = PCA()

pca.fit(X_train)

X_new = pca.transform(X_test)
```



Core API Summary

`estimator.fit(X, [y])`

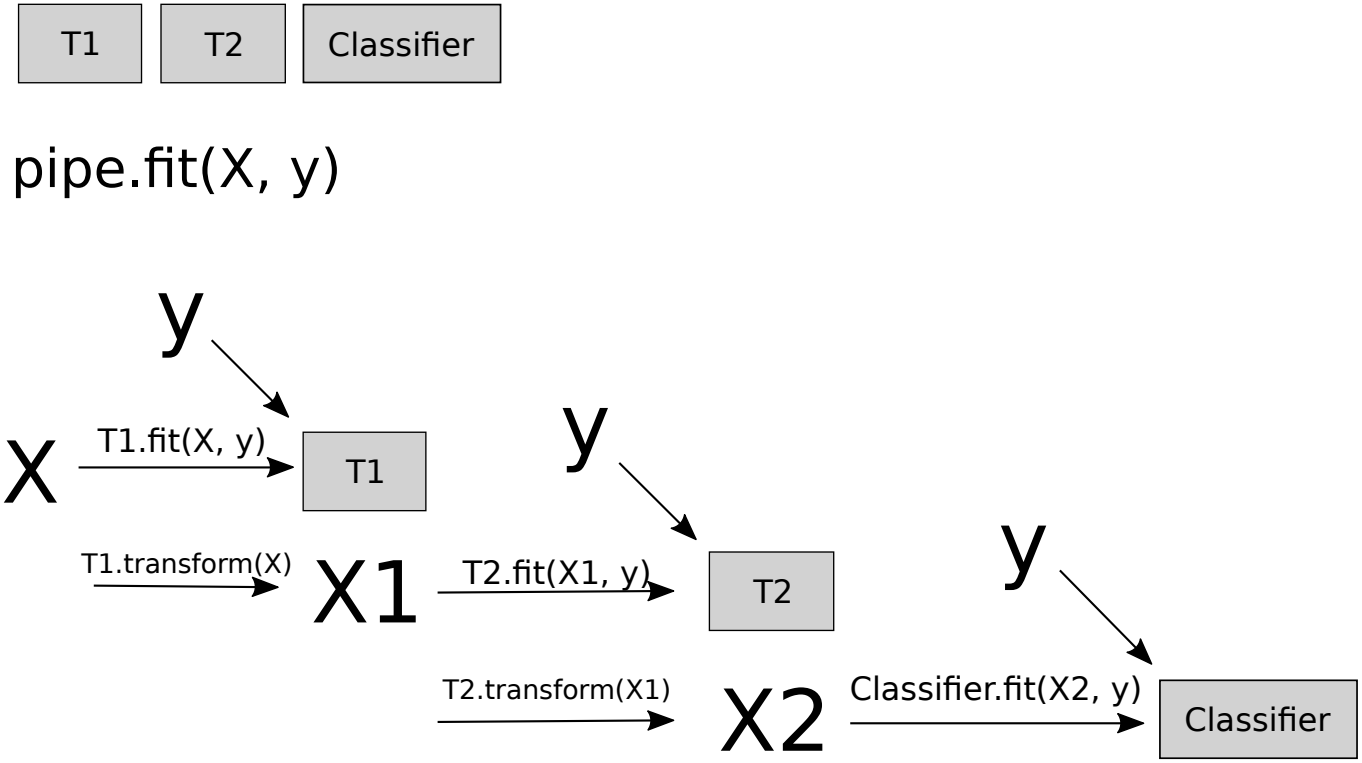
`estimator.predict`	`estimator.transform`
Classification	Preprocessing
Regression	Dimensionality reduction
Clustering	Feature selection
	Feature extraction

Cross -Validated Grid Search

```
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y)

param_grid = {'C': 10. ** np.arange(-3, 3),
              'gamma': 10. ** np.arange(-3, 3)}
grid = GridSearchCV(SVC(), param_grid=param_grid)
grid.fit(X_train, y_train)
grid.predict(X_test)
grid.score(X_test, y_test)
```

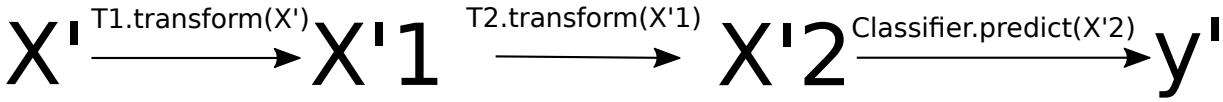
Pipelines

pipe = make_pipeline(T1(), T2(), Classifier())



pipe.fit(X, y)

pipe.predict(X')



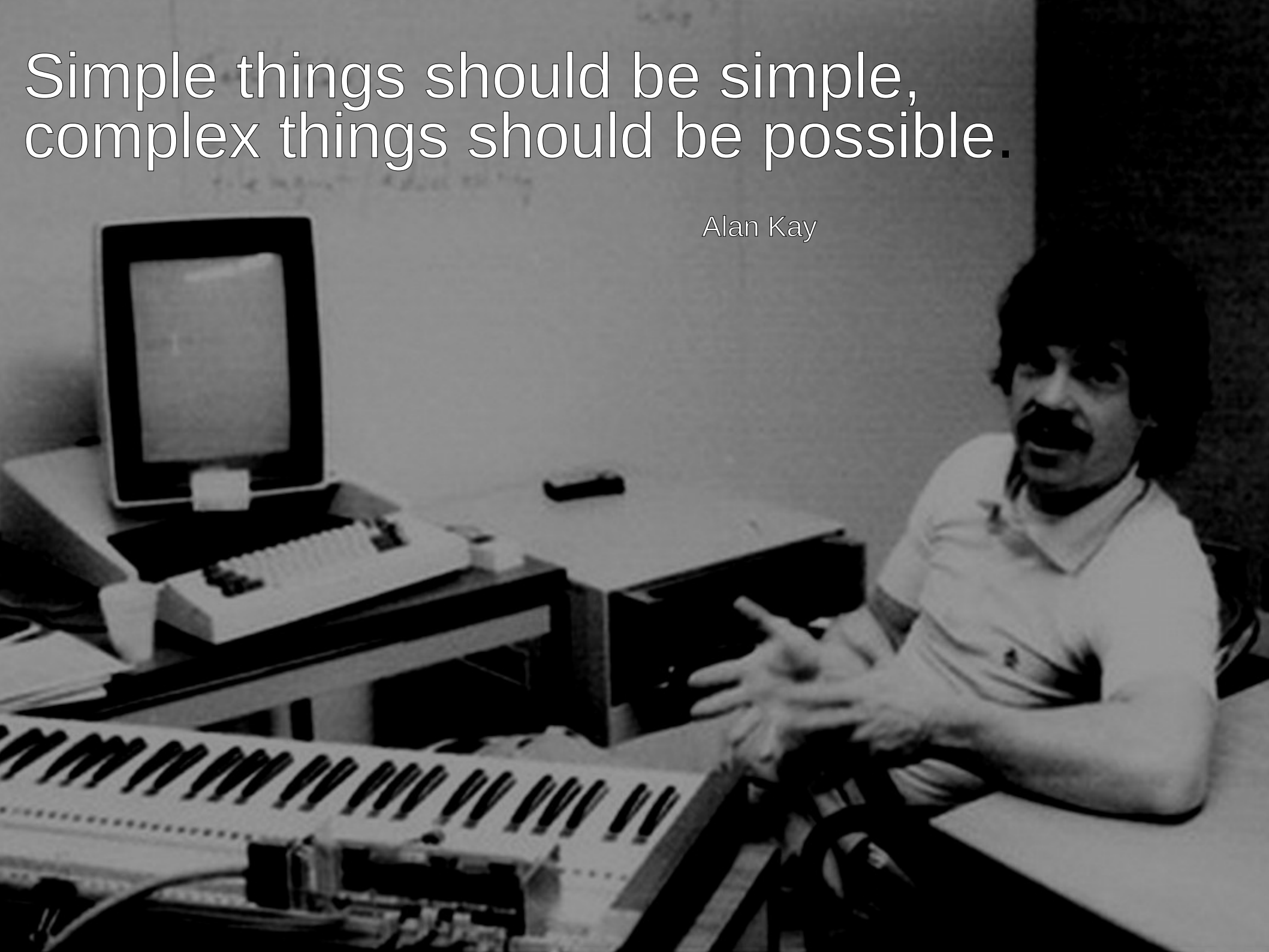
Pipelines

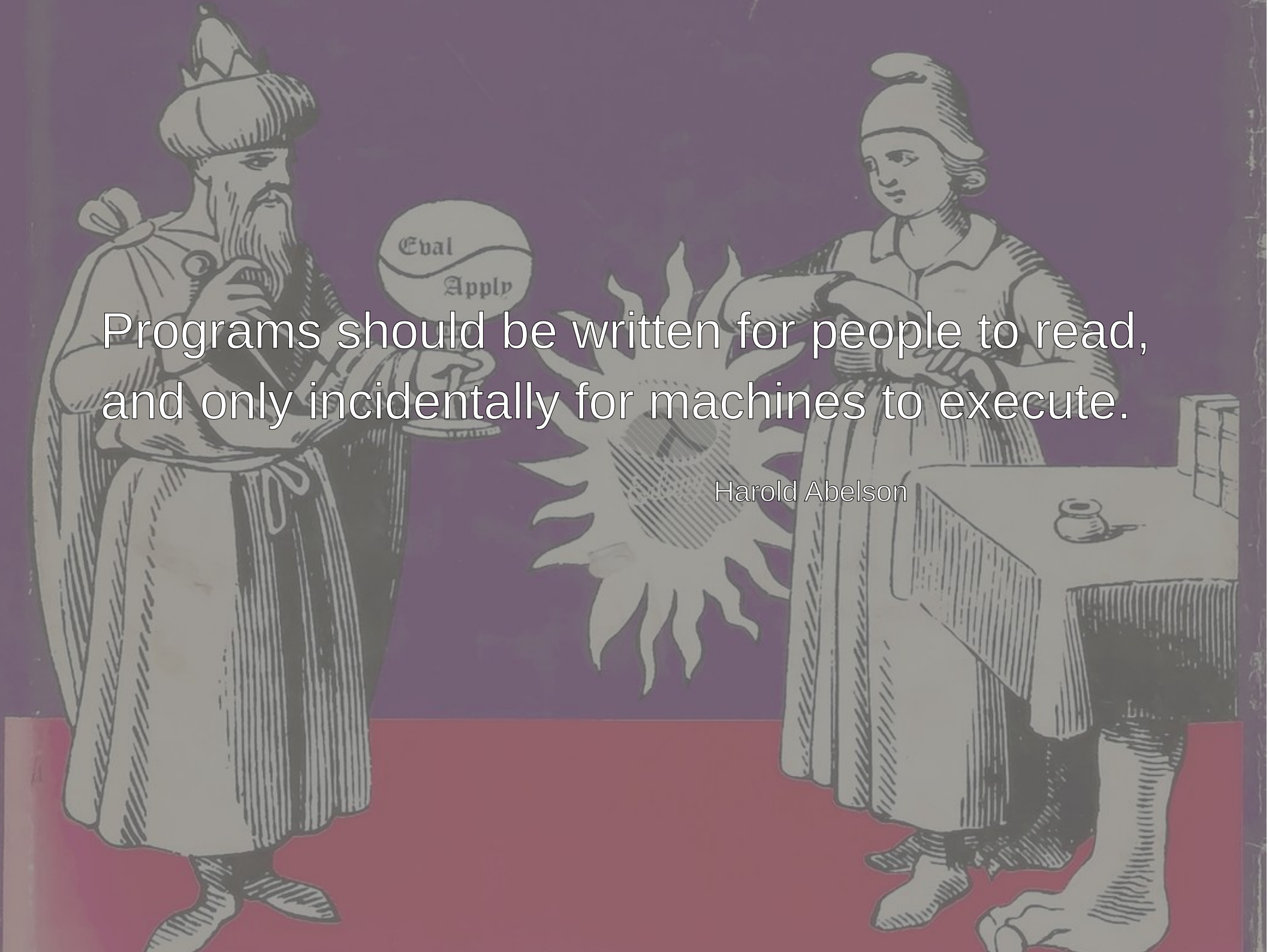
```
from sklearn.pipeline import make_pipeline

pipe = make_pipeline(StandardScaler(), SVC())
pipe.fit(X_train, y_train)
pipe.predict(X_test)
```

Guiding Ideas

Goals:

Maintainability
Ease of use


Simple things should be simple,
complex things should be possible.
Alan Kay



Programs should be written for people to read, and only incidentally for machines to execute.

Harold Abelson

Simplicity

```
lr = LogisticRegression()
lr.fit(X_train, y_train)
lr.score(X_test, y_test)
```

Consistency

```
grid = GridSearchCV(svm,param_grid)
grid.fit(X_train, y_train)
grid.score(X_test, y_test)
```

Composition

```
feature_selection = RFECV(NaiveBayes())
pipe = make_pipeline(feature_selection,
                     RandomForestClassifier())
grid = GridSearchCV(pipe, param_grid)
```

Default Parameters

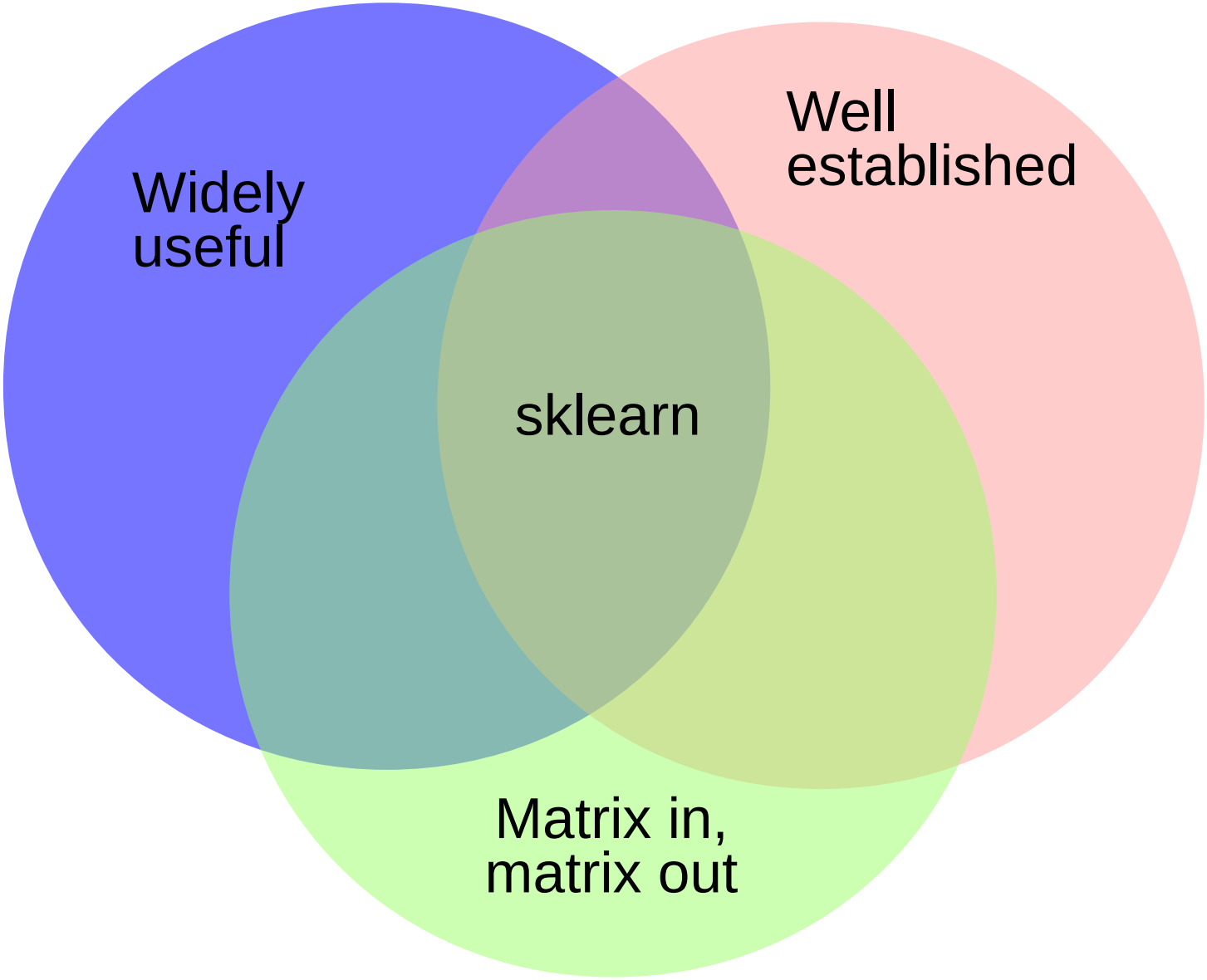
```
In [2]: clf = SVC()
        clf.fit(X_train, y_train)
```

```
SVC(self, C=1.0, kernel='rbf', degree=3, gamma=0.0, coef0=0.0,
 shrinking=True, probability=False, tol=0.001, cache_size=200,
 class_weight=None, verbose=False, max_iter=-1, random_state=N
one)
```

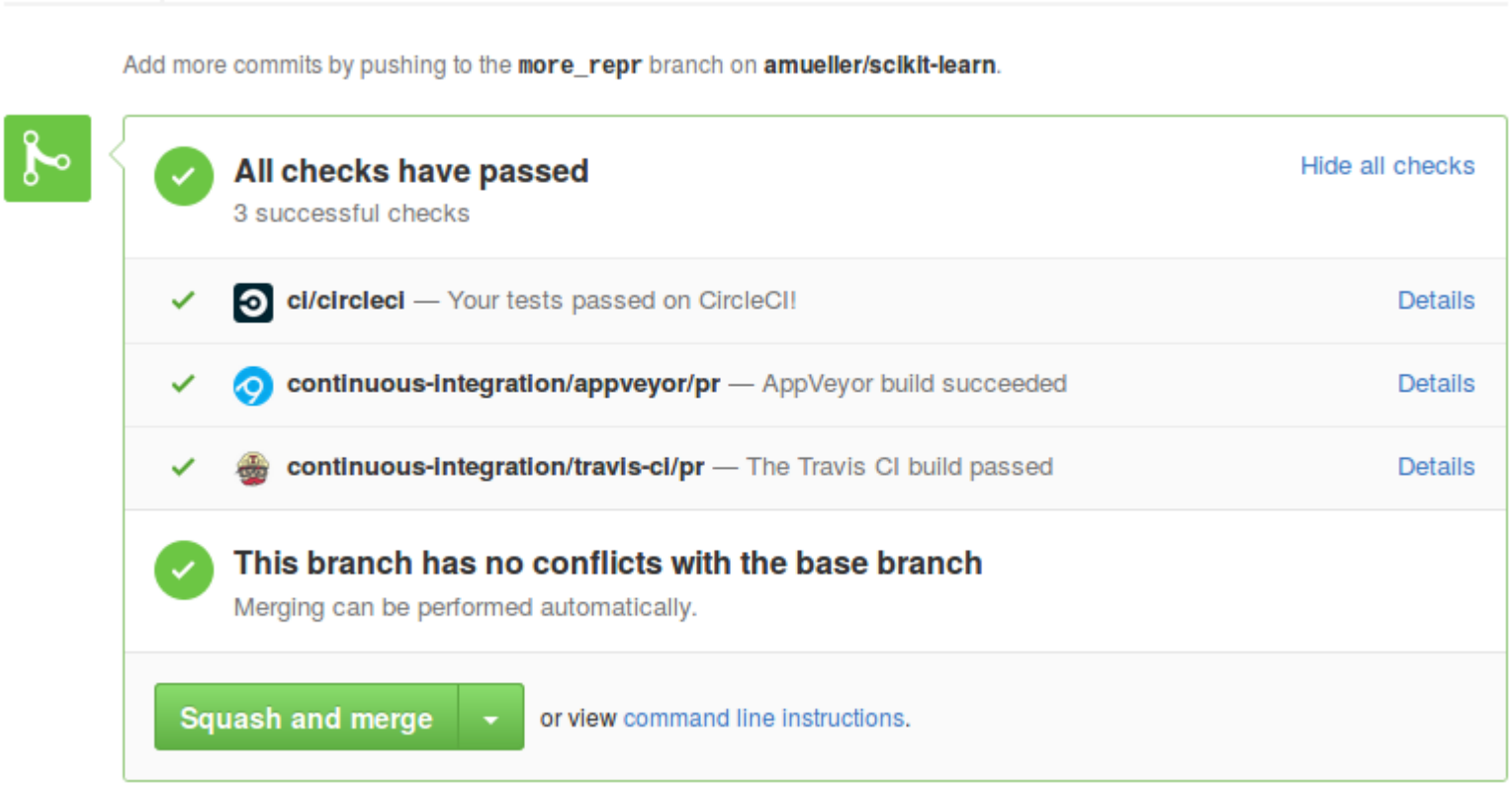
Flat Class Hierarchy, Few Types

- Numpy arrays / sparse matrices
- Estimators
- Cross-validation objects
- Scorers

Scoping


Widely
useful
Well
established
sklearn
Matrix in,
matrix out

Testing & Continuous Integration



Three way documentation

1.9. Ensemble methods

The goal of **ensemble methods** is to combine the predictions of several base estimators built with a given learning algorithm in order to improve generalizability / robustness over a single estimator.

Two families of ensemble methods are usually distinguished:

- In **averaging methods**, the driving principle is to build several estimators independently and then to average their predictions. On average, the combined estimator is usually better than any of the single base estimator because its variance is reduced.

  Examples: *Bagging methods*, *Forests of randomized trees*, ...
- By contrast, in **boosting methods**, base estimators are built sequentially and one tries to reduce the bias of the combined estimator. The motivation is to combine several weak models to produce a powerful ensemble.

  Examples: *AdaBoost*, *Gradient Tree Boosting*, ...

`sklearn.ensemble`.RandomForestClassifier

class `sklearn.ensemble.` **`RandomForestClassifier`** (*n_estimators=10, criterion='gini', max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features='auto', max_leaf_nodes=None, bootstrap=True, oob_score=False, n_jobs=1, random_state=None, verbose=0, warm_start=False*) [source]

A random forest classifier.

A random forest is a meta estimator that fits a number of decision tree classifiers on various sub-samples of the dataset and use averaging to improve the predictive accuracy and control over-fitting.

Parameters:

n_estimators : integer, optional (default=10)

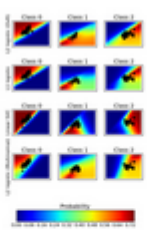
The number of trees in the forest.

criterion : string, optional (default="gini")

The function to measure the quality of a split. Supported criteria are "gini" for the Gini impurity and "entropy" for the information gain. Note: this parameter is tree-specific.

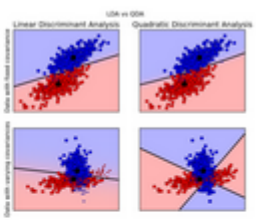
Examples

Recognizing hand-written digits



Plot classification probability

Classifier comparison



Linear and Quadratic Discriminant Analysis with confidence ellipsoid

Behind the scenes

API implementation & contracts

Method Chaining

Fit must return self:

```
X_scaled = StandardScaler().fit(X).transform(X)

pred = SVC().fit(X_train, y_train).score(
    X_test, y_test)
```

fit resets

```
from sklearn.tree import DecisionTreeClassifier
tree = DecisionTreeClassifier(max_depth=10)
tree.fit(iris.data, iris.target)
score_iris = tree.score(iris.data, iris.target)
tree.fit(digits.data, digits.target)
score_digits = tree.score(digits.data, digits.target)
```

__init__ does nothing

```
class PCA():
    def __init__(self, n_components=None, copy=True, whiten=False,
                 svd_solver='auto', tol=0.0, iterated_power='auto',
                 random_state=None):
        self.n_components = n_components
        self.copy = copy
        self.whiten = whiten
        self.svd_solver = svd_solver
        self.tol = tol
        self.iterated_power = iterated_power
        self.random_state = random_state
```

get_params & set_params

```
def get_params(self, deep=True):
    out = dict()
    for key in signature(self.__init__):
        value = getattr(self, key, None)
        if deep and hasattr(value, 'get_params'):
            deep_items = value.get_params().items()
            out.update((key + '__' + k, val) for k, val in deep_items)
        out[key] = value
    return out
```

Used in GridSearchCV etc.
Not __init__ !!!
All parameter validation etc in fit!

(only) fit mutates self

- __init__ only remembers construction parameters
- Transform / score etc don’t change object
- Fit returns self but mutates object!

Estimated attributes

```
Attributes
----------
components_ : array, shape (n_components, n_features)
    Principal axes in feature space, representing the directions of
    maximum variance in the data. The components are sorted by
    ``explained_variance_``.

explained_variance_ : array, shape (n_components,)
    The amount of variance explained by each of the selected components.

    Equal to n_components largest eigenvalues
    of the covariance matrix of X.

    .. versionadded:: 0.18

explained_variance_ratio_ : array, shape (n_components,)
    Percentage of variance explained by each of the selected components.

    If ``n_components`` is not set then all components are stored and the
    sum of the ratios is equal to 1.0.

singular_values_ : array, shape (n_components,)
    The singular values corresponding to each of the selected components.
    The singular values are equal to the 2-norms of the ``n_components``
    variables in the lower-dimensional space.
```

Leaves two kinds of attributes:
arguments to __init__; things estimated during fit

fit_transform / fit_predict

In general: computational shortcut:

```
pca = PCA()
pca.fit(X)
X_pca = pca.transform(X)
X_pca2 = pca.fit_transform(X)
```

Clustering / Manifold learning: Not inductive.

```
tsne = TSNE()
X_tsne = tsne.fit_transform(X)
```

```
dbscan = DBSCAN()
cluster_labels = dbscan.fit_predict(X)
```

check_estimator

```python
class TemplateClassifier(BaseEstimator, ClassifierMixin):

    def __init__(self, demo_param='demo'):
        self.demo_param = demo_param

    def fit(self, X, y):

        # Check that X and y have correct shape
        X, y = check_X_y(X, y)
        # Store the classes seen during fit
        self.classes_ = unique_labels(y)

        self.X_ = X
        self.y_ = y
        # Return the classifier
        return self

    def predict(self, X):

        closest = np.argmin(euclidean_distances(X, self.X_), axis=1)
        return self.y_[closest]
```

```python
check_estimator(TemplateClassifier)
```

```
AssertionError: Error message does not include the expected string: 'fit'.
Observed error message: "'TemplateClassifier' object has no attribute 'X_'"
```

Other API Building Blocks

Scorers

```
grid = GridSearchCV(SVC(), params, scoring='roc_auc')

def my_acc_scorer(est, X, y):
    y_pred = est.predict(X)
    return (y == y_pred).mean()

grid = GridSearchCV(SVC(), params,
                    scoring=my_acc_scorer)
```

Cross-validation iterators

```
grid = GridSearchCV(SVC(), param_grid, cv=5)

cv = KFold(n_split=5, shuffle=True, random_state=3)

grid = GridSearchCV(SVC(), param_grid, cv=cv)


cv = RepeatedKFold(n_split=5, n_repeats=10)
grid = GridSearchCV(SVC(), param_grid, cv=cv)
```

CV Iterators API

```
def split(self, X, y=None, groups=None):
    """Generate indices to split data into training and test set.

    Parameters
    ----------
    X : array-like, shape (n_samples, n_features)
        Training data, where n_samples is the number of samples
        and n_features is the number of features.

    y : array-like, of length n_samples
        The target variable for supervised learning problems.

    groups : array-like, with shape (n_samples,), optional
        Group labels for the samples used while splitting the dataset into
        train/test set.

    Returns
    -------
    train : ndarray
        The training set indices for that split.

    test : ndarray
        The testing set indices for that split.
    """
```

```
kfold = KFold(n_splits=5)
for train, test in kfold.split(X, y):
    X_train = X[train]
    X_test = X[test]
```

Misc functions

- Scoring functions
  func(y_true, y_pred/y_scores, …)

- Pairwise Distances/kernels

  euclidean_distances
  rbf_kernel

- Evaluation:
  cross_validate
  learning_curve
  roc_curve

- Helpers:
  train_test_split

Development Practices

Standards for OSS

Everything discussed in the open.
Every convention and process documented.

Development guide

http://scikit-learn.org/dev/developers/contributing.html

Contains:

- API details
- Bug report guidelines
- PR guidelines
- Reviewing guidelines
- How to find issues
- Details of CI

Even more at http://scikit-learn.org/dev/developers/

Sphinx / numpydoc

```
class MultinomialNB(BaseDiscreteNB):
    """
    Naive Bayes classifier for multinomial models

    The multinomial Naive Bayes classifier is suitable for classification with
    discrete features (e.g., word counts for text classification). The
    multinomial distribution normally requires integer feature counts. However,
    in practice, fractional counts such as tf-idf may also work.

    Read more in the :ref:`User Guide <multinomial_naive_bayes>`.

    Parameters
    ----------
    alpha : float, optional (default=1.0)
        Additive (Laplace/Lidstone) smoothing parameter
        (0 for no smoothing).

    fit_prior : boolean, optional (default=True)
        Whether to learn class prior probabilities or not.
        If false, a uniform prior will be used.

    class_prior : array-like, size (n_classes,), optional (default=None)
        Prior probabilities of the classes. If specified the priors are not
        adjusted according to the data.

    Attributes
    ----------
    class_log_prior_ : array, shape (n_classes, )
        Smoothed empirical log probability for each class.

    intercept_ : property
        Mirrors ``class_log_prior_`` for interpreting MultinomialNB
        as a linear model.

    feature_log_prob_ : array, shape (n_classes, n_features)
        Empirical log probability of features
        given a class, ``P(x_i|y)``.

    coef_ : property
        Mirrors ``feature_log_prob_`` for interpreting MultinomialNB
        as a linear model.

    class_count_ : array, shape (n_classes,)
        Number of samples encountered for each class during fitting. This
        value is weighted by the sample weight when provided.

    feature_count_ : array, shape (n_classes, n_features)
        Number of samples encountered for each (class, feature)
        during fitting. This value is weighted by the sample weight when
        provided.

    Examples
    --------
    >>> import numpy as np
    >>> X = np.random.randint(5, size=(6, 100))
    >>> y = np.array([1, 2, 3, 4, 5, 6])
    >>> from sklearn.naive_bayes import MultinomialNB
    >>> clf = MultinomialNB()
    >>> clf.fit(X, y)
    MultinomialNB(alpha=1.0, class_prior=None, fit_prior=True)
    >>> print(clf.predict(X[2:3]))
    [3]

    Notes
    -----
    For the rationale behind the names `coef_` and `intercept_`, i.e.
    naive Bayes as a linear classifier, see J. Rennie et al. (2003),
    Tackling the poor assumptions of naive Bayes text classifiers, ICML.

    References
    ----------
    C.D. Manning, P. Raghavan and H. Schuetze (2008). Introduction to
    Information Retrieval. Cambridge University Press, pp. 234-265.
    http://nlp.stanford.edu/IR-book/html/htmledition/naive-bayes-text-classification-1.html
    """
```

sklearn.naive_bayes.MultinomialNB

class sklearn.naive_bayes.**MultinomialNB**(*alpha=1.0, fit_prior=True, class_prior=None*) [source]

Naive Bayes classifier for multinomial models

The multinomial Naive Bayes classifier is suitable for classification with discrete features (e.g., word counts for text classification). The multinomial distribution normally requires integer feature counts. However, in practice, fractional counts such as tf-idf may also work.

Read more in the User Guide.

Parameters:

alpha : *float, optional (default=1.0)*
Additive (Laplace/Lidstone) smoothing parameter (0 for no smoothing).

fit_prior : *boolean, optional (default=True)*
Whether to learn class prior probabilities or not. If false, a uniform prior will be used.

class_prior : *array-like, size (n_classes,), optional (default=None)*
Prior probabilities of the classes. If specified the priors are not adjusted according to the data.

Attributes:

class_log_prior_ : *array, shape (n_classes,)*
Smoothed empirical log probability for each class.

intercept_ : *array, shape (n_classes,)*
Mirrors `class_log_prior_` for interpreting MultinomialNB as a linear model.

feature_log_prob_ : *array, shape (n_classes, n_features)*
Empirical log probability of features given a class, `P(x_i|y)`.

coef_ : *array, shape (n_classes, n_features)*
Mirrors `feature_log_prob_` for interpreting MultinomialNB as a linear model.

class_count_ : *array, shape (n_classes,)*
Number of samples encountered for each class during fitting. This value is weighted by the sample weight when provided.

feature_count_ : *array, shape (n_classes, n_features)*
Number of samples encountered for each (class, feature) during fitting. This value is weighted by the sample weight when provided.

Notes

For the rationale behind the names coef_ and intercept_, i.e. naive Bayes as a linear classifier, see J. Rennie et al. (2003), Tackling the poor assumptions of naive Bayes text classifiers, ICML.

References

C.D. Manning, P. Raghavan and H. Schuetze (2008). Introduction to Information Retrieval. Cambridge University Press, pp. 234-265. http://nlp.stanford.edu/IR-book/html/htmledition/naive-bayes-text-classification-1.html

Examples

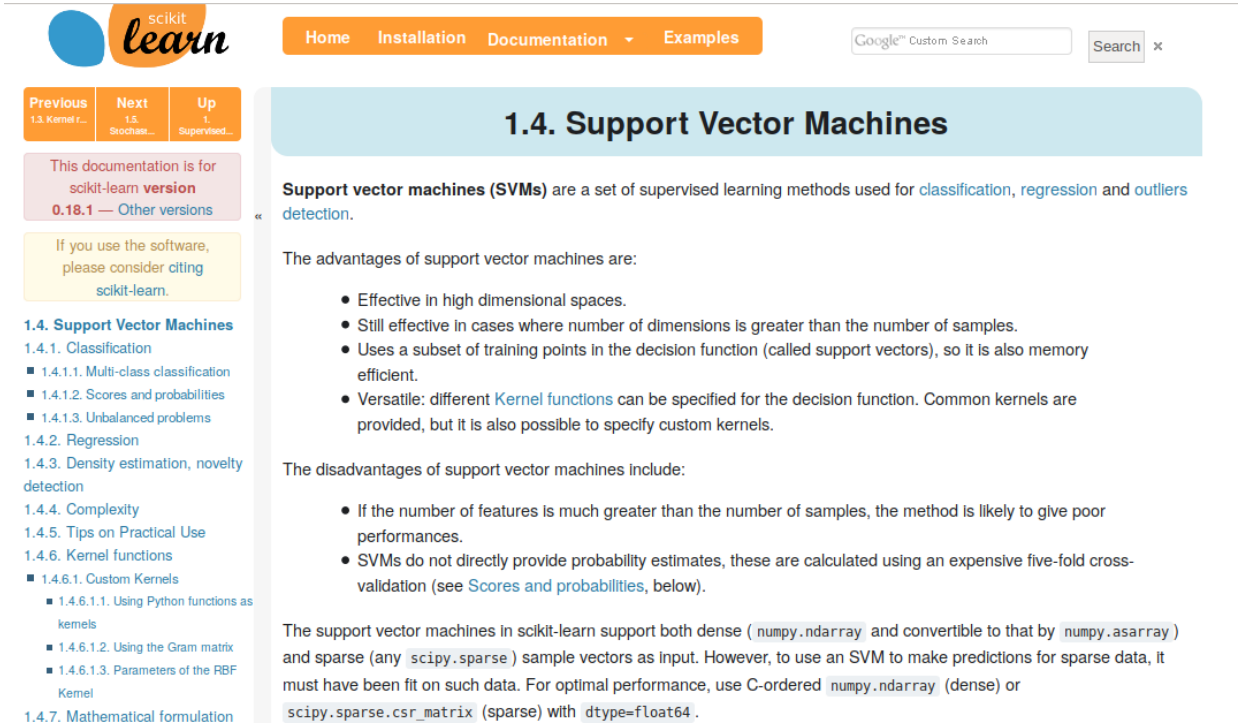
```
>>> import numpy as np
>>> X = np.random.randint(5, size=(6, 100))
>>> y = np.array([1, 2, 3, 4, 5, 6])
>>> from sklearn.naive_bayes import MultinomialNB
>>> clf = MultinomialNB()
>>> clf.fit(X, y)
MultinomialNB(alpha=1.0, class_prior=None, fit_prior=True)
>>> print(clf.predict(X[2:3]))
[3]
```

Methods

`fit`(X, y[, sample_weight])	Fit Naive Bayes classifier according to X, y
`get_params`([deep])	Get parameters for this estimator.
`partial_fit`(X, y[, classes, sample_weight])	Incremental fit on a batch of samples.
`predict`(X)	Perform classification on an array of test vectors X.
`predict_log_proba`(X)	Return log-probability estimates for the test vector X.
`predict_proba`(X)	Return probability estimates for the test vector X.
`score`(X, y[, sample_weight])	Returns the mean accuracy on the given test data and labels.
`set_params`(**params)	Set the parameters of this estimator.

Sphinx / numpydoc

```
.. _svm:

=======================
Support Vector Machines
=======================

.. currentmodule:: sklearn.svm

**Support vector machines (SVMs)** are a set of supervised learning
methods used for :ref:`classification <svm_classification>`,
:ref:`regression <svm_regression>` and :ref:`outliers detection
<svm_outlier_detection>`.

The advantages of support vector machines are:

    - Effective in high dimensional spaces.

    - Still effective in cases where number of dimensions is greater
      than the number of samples.

    - Uses a subset of training points in the decision function (called
      support vectors), so it is also memory efficient.

    - Versatile: different :ref:`svm_kernels` can be
      specified for the decision function. Common kernels are
      provided, but it is also possible to specify custom kernels.

The disadvantages of support vector machines include:

    - If the number of features is much greater than the number of
      samples, the method is likely to give poor performances.

    - SVMs do not directly provide probability estimates, these are
      calculated using an expensive five-fold cross-validation
      (see :ref:`Scores and probabilities <scores_probabilities>`, below).

The support vector machines in scikit-learn support both dense
(``numpy.ndarray`` and convertible to that by ``numpy.asarray``) and
sparse (any ``scipy.sparse``) sample vectors as input. However, to use
an SVM to make predictions for sparse data, it must have been fit on such
data. For optimal performance, use C-ordered ``numpy.ndarray`` (dense) or
``scipy.sparse.csr_matrix`` (sparse) with ``dtype=float64``.
```



Deprecations / backward compatibility

- Don’t change any behavior (except bug fixes)

```
@property
@deprecated("Attribute labels_ was deprecated in version 0.13 and "
            "will be removed in 0.15. Use 'classes_' instead")
def labels_(self):
    return self.classes_
```

Practical Notes on Contributing

Describing PR

Open a pull request

Create a new pull request by comparing changes across two branches. If you need to, you can also compare across forks.

base fork: **scikit-learn/scikit-learn** | base: **master** | ... | head fork: **amueller/scikit-learn** | compare: **my_feature_branch** | ✓ **Able to merge.** These br

Please review the **guidelines for contributing** to this repository.

[WIP] = work in progress
[MRG] = ready to merge

[MRG] minor pep8

Write | Preview

```
<!--
Thanks for contributing a pull request! Please ensure you have taken a look at
the contribution guidelines: https://github.com/scikit-learn/scikit-learn/blob/master
/CONTRIBUTING.md#Contributing-Pull-Requests
-->
### Reference Issue
<!-- Example: Fixes #1234 -->
```

Attach files by dragging & dropping, selecting them, or pasting from the clipboard.

Allow edits from maintainers. Learn more

Create pull request

Reviewers
No reviews—request one

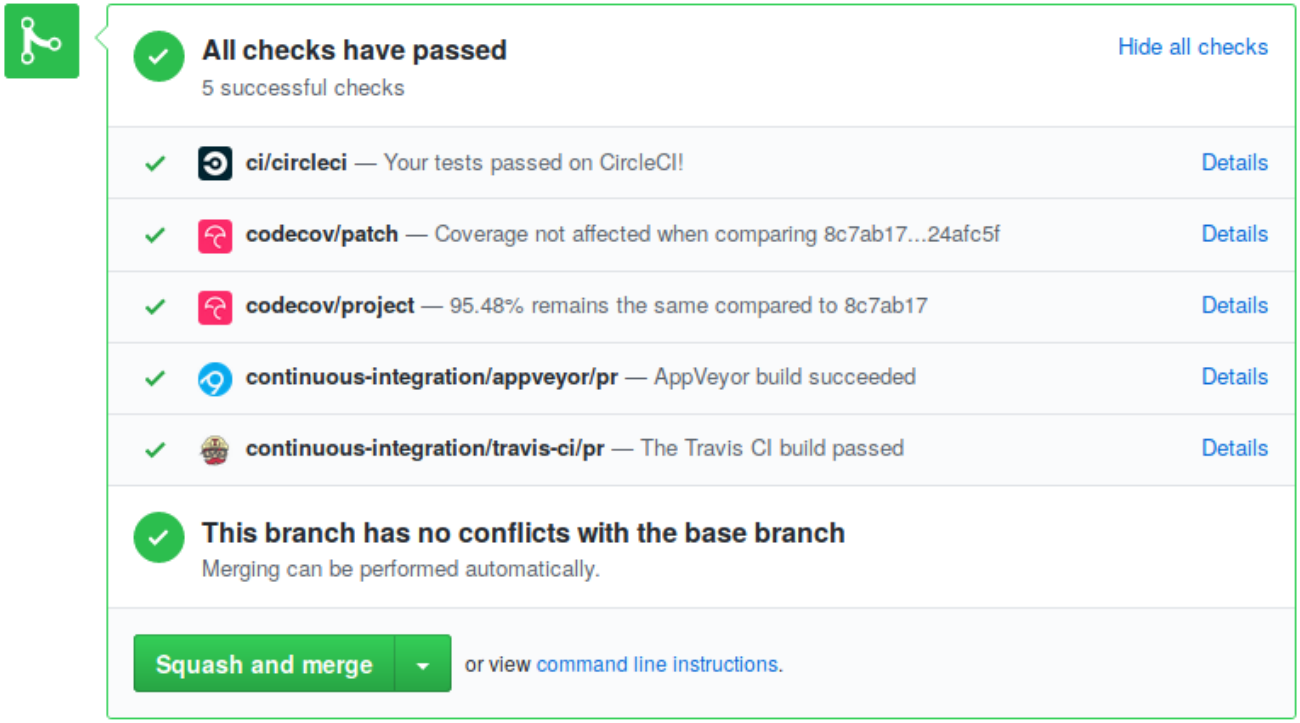
Assignees
No one—assign yourself

Labels
None yet

Milestone
No milestone

Regression tests

- Are mandatory! For everything (except documentation changes)!
- Make sure continuous integration passes:



What's next?

- Wait for reviews (be patient).
- Address review comments in the same branch.
- Pushing to your fork will update the PR
- Reviewers will "approve" PR or change title to [MRG + 1]
- You need two approvals for a merge.

Finding Issues

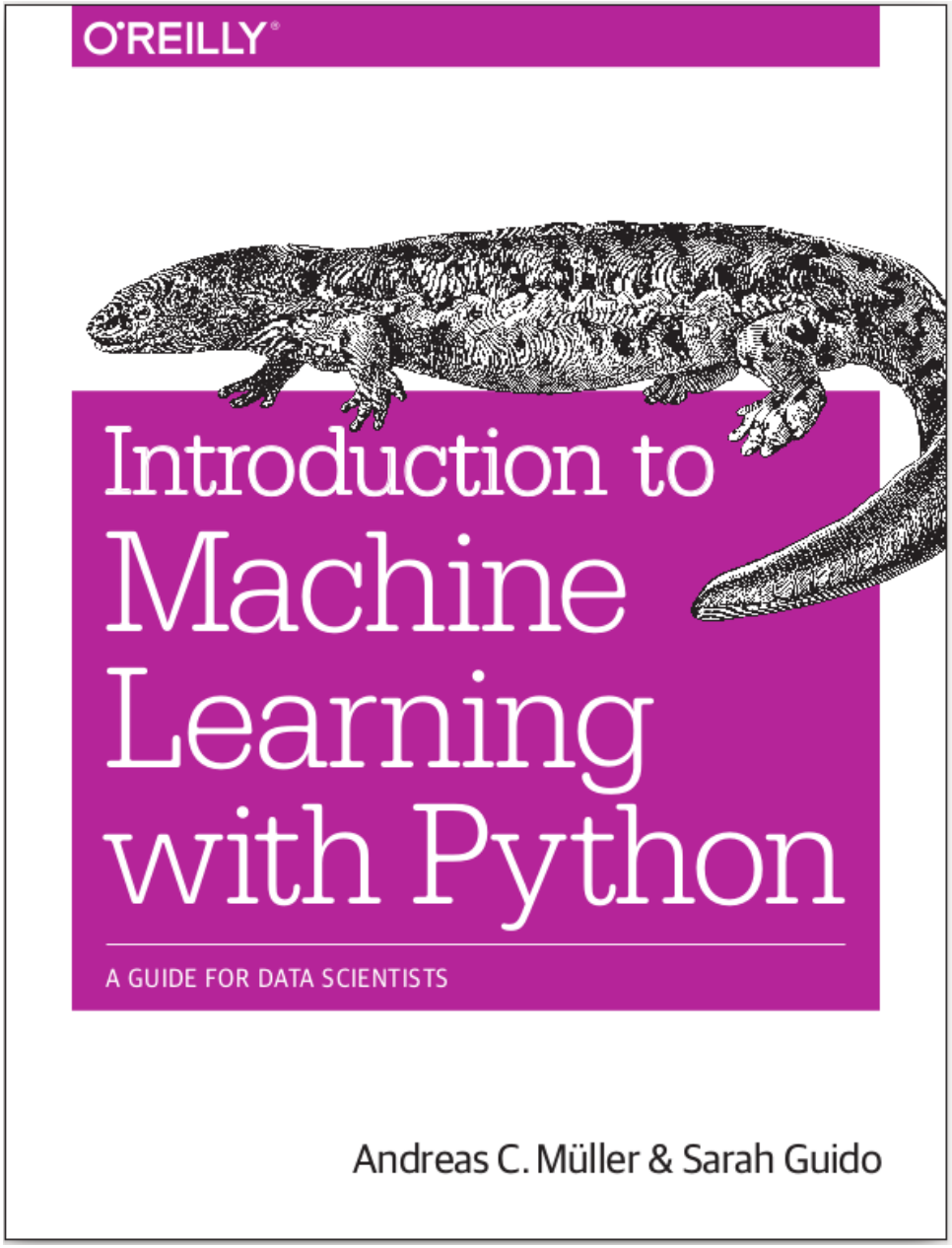
- Check “need contributor”, “easy” and “sprint” issues.
- Something unclear in the docs? Fix it!
- Can’t fix something that’s unclear? Open an issue!
- Problem that you keep running into: Open an issue!
- Find stalled PRs (the author didn’t address reviews for ~>1 month) and continue them!

Reviewing

- You can review PRs and issues!
- Some bugs are not confirmed. See if you can confirm them and under what conditions?
- You can review documentation PRs for language and whether they are clear to you.
- You can review code changes on whether they address the issue (might be a bit tricky).
- Don't be afraid to ask clarifying questions!

Final words

- Pick something TRIVIALLY SIMPLE as the first contribution.
- You can do the cool stuff afterwards!
- There might be interesting issues that are not appropriately tagged.
- Consider finishing up stalled PRs


O'REILLY
Introduction to
Machine
Learning
with Python
A GUIDE FOR DATA SCIENTISTS
Andreas C. Müller & Sarah Guido

Thank you.

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http://amueller.io